

Theoretical Studies of New High Explosive Materials: N₄

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In the field of high explosives and propellants it is desirable to produce a dense material that releases a lot of energy through highly exothermic chemical reactions. We have begun a first-principles investigation of the N₄ molecule as an energetic material that may exhibit these desired properties through the reaction



We are currently investigating the energy barrier for decomposition of N₄ in the gas phase by making use of a multiconfigurational quantum mechanical

method in which the electrons in the highest occupied 12 orbitals are excited into the 12 lowest unoccupied orbitals.

In addition, we are making use of solid-state quantum mechanical methods to explore possible crystal packing structures of N₄ and their shock-inducing decomposition.

As shown in the figure, this chemical reaction releases a generous amount of energy making N₄ materials worthy of further study.

We have begun a first-principles investigation of the N₄ molecule as a prospective energetic material.

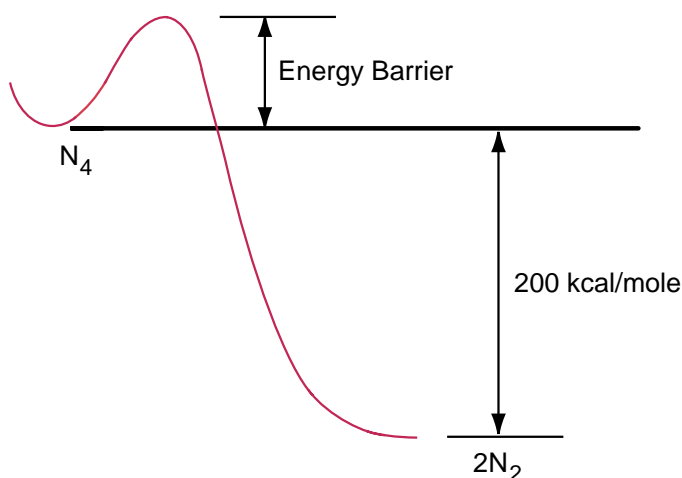


Figure: Current work is focusing on determining the energy barrier for this reaction in the gas phase and on finding the density of its crystalline structure using solid-state density-functional computational methods.